

Workshops are organized on topics of special interest with a focus on new technology.
There is no additional charge for workshops – they are open to all as a forum for discussion.

MONDAY WORKSHOPS, 5:45 – 7:00 PM**Tips and Tricks for the MS Analysis of Nucleic Acids and their Assemblies***DNA/RNA Interest Group*

D. Fabris and V. Gabelica, presiding

The workshop will cover the practical aspects of MS analysis of nucleic acids by MALDI and ESI. A panel of experts will provide tips on how to overcome the challenges posed by the characterization of covalent and non-covalent adducts and will address questions raised by the audience.

Integrated Quantitative and Qualitative LC-MS Approaches: Revisiting with New Technologies*Drug Metabolism and Pharmacokinetics Interest Group*

Lucinda Cohen and Ragu Ramanathan, presiding

Workshop will include a panel discussion on the utility of high resolution and fast scanning mass spectrometer based approaches for integrating quantitative and qualitative LC-MS approaches for assessing DMPK properties. LC-MS approaches to acquire metabolite information early in the discovery program as well as in early clinical studies will be discussed by industry leaders. Time for lively discussion is included. Meeting will open with brief discussion on DMPK Interest Group impact on 2009 conference program and request for suggestions on 2010 session, and workshop topics. New DMPK-IG officers will also be elected at this meeting.

FTMS*FTMS Interest Group*

Yury O. Tsybin, presiding

In-depth understanding of ion behavior in traps and induced current generation principles are the basis of recent improvements of high resolution mass spectrometry performance. We will discuss these and other advances in FTMS instrumentation and fundamentals, as well as current limitations, in a workshop format meeting. In addition, last minute hot topics are welcome to the stage in the usual format of short presentation.

Metal Ions in the Gas Phase*Metal Ion Coordination Chemistry Interest Group*

Victor Ryzhov, presiding

This workshop will encompass various topics involving gas-phase metal ions (bare and coordinated), including challenges in metal ion formation, their reactivity, structure and energetics. Sample topics include: Thermochemistry of metal-ligand binding, structure of metal complexes, metal ion reactivity, role of metal ions in gas-phase catalysis. Discussion will also be held on the advantages of using metal ions to enhance/influence dissociation of biomolecules. Approaches complementary to the experimental mass spectrometry techniques (such as theoretical calculations and ion spectroscopy) will be presented as well.

NCI-Clinical Proteomics Technology Assessment in Cancer

Steve Carr, presiding

Glycomics and Glycoproteomics: How Challenging

Yehia Mechref, presiding

Structural characterization of biologically important oligosaccharides has been increasingly emphasized, since it appears that most of the processes in the living cells are associated with different forms of carbohydrate interactions. Glycosylation of proteins and the interactions of glycans and other biomolecular entities touch on many areas of modern biology and medicine. Any alterations in a glycan composition or structure could potentially be either a cause or consequential attributes of the biochemical in balance that is recognized as a “disease”. Although the development of different structural tools (the majority of which based on mass spectrometry) has somewhat paved the way to a better understanding of oligosaccharide roles in signaling and regulations between various cells, the inherent difficulties of structural analysis in glycobiology still exist. These difficulties mainly originate from (a) structural complexity of glycoconjugates featuring various forms of branching and other types of isomerism; (b) microheterogeneities at the sites of glycosylation; (c) extensive occurrence of glycosylation in eukaryotic proteins; and (d) distribution of glycosylated proteins in different parts of living cells. This workshop will highlight these challenging aspects and describe the state-of-the-art approaches and their applications in biology and medicine.

TUESDAY WORKSHOPS, 5:45 – 7:00 PM

Mass Spectrometry Applications in Clinical Diagnostics: From the Bench to the Bedside*Clinical Chemistry Interest Group*

Russell Grant and Nigel Clarke, presiding

This interactive workshop will highlight and discuss the 2 different routes from inception of a MS based diagnostic assay to clinical utility. The first route will involve discussion regarding conversion of established clinical biomarkers to MS technologies. Validation criteria and standardization efforts will be discussed. The second route will discuss new biomarker panels with a view towards FDA submissions and the IVDMA process. Brief presentation vignettes (2-3 slides from 3-4 speakers maximum) from industry and government representatives will be used to initiate discussions.

Identification of Counterfeit Foods and Ingredients by Mass Spectrometry*Flavor, Fragrance and Foodstuff Interest Group*

David Heller, presiding

Mass spectrometry plays a variety of roles in the detection of counterfeit food and flavor ingredients. The workshop aims to bring together analysts with an interest in this broad application area, which can include enforcement of product specifications and safety standards, detection of substitutes or contaminants, determining location or species of origin, forensic analysis, or use in regulatory action. The workshop will include examples as well as discussion of recent developments, current needs and concerns. Attendees are invited to share problem-solving techniques and to identify issues

How Hot Is your Mass Spectrometer?*Fundamentals Interest Group*

Elaine Marzluff, presiding

Many mass spectrometry experiments assume an energy distribution of ions in a mass spectrometer, but knowing that energy distribution can be quite challenging. In this workshop we will consider what is known about some fundamental ways of knowing the temperature distribution of ions, and results for several types of mass spectrometers and ion sources.

Current Topics in Metabolomics*Metabolomics Interest Group*

Eric Milgram and Anders Nordstrom, presiding

A WWW-based survey was conducted in order to determine which metabolomics topics are of the most interest to workshop participants. Survey aspects included where the technique is being applied, the types of instrumentation and software being used, as well as metabolite identification and assignment of biological significance. The data from the survey was used to determine which topics should be covered for this year's workshop. In addition to discussing the results of the survey, there will be interactive discussions based on the survey results.

Advances, Applications, and Limitations of Accurate Mass Measurements*Pharmaceuticals Interest Group*

Chris Petucci and Carmen Santasania, presiding

Recent advances in accurate mass instrumentation have made sub-ppm mass accuracy routinely attainable in drug discovery and development. This workshop will be a panel led discussion to discuss the current applications of accurate mass instrumentation in the pharmaceutical industry. In addition, highlights of a survey to benchmark the current industry practices with accurate mass instrumentation will be discussed.

Polymer Problem Solving Session and Interest Group Meeting*Polymeric Materials Interest Group*

Michael Polce, presiding

The workshop will consist of several short informal presentations (3-5 slides) in which speakers briefly describe a specific unresolved measurement challenge they have encountered (sample prep, ionization issues, data interpretation, etc.) and the audience provides useful comments and suggestions in an open discussion. A brief meeting will follow to discuss any technical topics of current interest to the group.

Challenge in LC-MS/MS Bioanalysis: Ion Suppression, Matrix Effect, Contamination Criteria and Regression Type*Regulated Bioanalysis Interest Group*

Fabio Garofolo, presiding

As per the input of the numerous interest group members who answered the Feb. 2009 survey, this year workshop will focus on the following 3 most requested "hot topics": 1) *Ion suppression and matrix effect: Do we need full or partial validation for the same compound in different species?* 2) *Contamination Criteria in LC-MS/MS: What criteria are you using?* 3) *Acceptance of nonlinear calibration models in LC-MS/MS: How much "quadratic" is acceptable?*

The purpose of this workshop is to provide an educational forum to discuss issues and applications associated with the LC-MS/MS Bioanalysis. The scientific debate will be led by three panelists who are recognized international experts in the field. They will introduce each of the above mentioned topics to engage the audience and encourage all to participate in a dynamic and productive discussion. The workshop report will be posted on the ASMS Regulated Bioanalysis Forum

Probing Protein Conformation - What's New?*H/D Exchange and Covalent Labeling Interest Group*

John R. Engen and Robert L. Hettich, presiding

The latest innovations in labeling strategies for understanding protein conformation and interactions will be discussed. Several hot topics in both H/D exchange and covalent labeling will be covered. The meeting will conclude with a software "free-for-all" where recent advances, challenges and solutions will be shown and explored.

WEDNESDAY WORKSHOPS, 5:45 – 7:00 PM**Finding Unknowns in the Environment: High Resolution and MS/MS Approaches***Environmental Applications Interest Group*

Enrico Davoli, presiding

High resolution MS is providing an extremely powerful tool for screening and identification of unknowns. Highly accurate data can be now easily obtained from TOF instruments, orbitraps and FT-ICR. Libraries and different types of data mining are available, but a standardized method is still lacking.

MS Applications in Forensics and Homeland Protection*Forensics and Homeland Security Interest Group*

Plamen A. Demirev, presiding

MS approaches for detection and identification of explosives, chemical and biological agents will be discussed. These will include specific methods for ionization, data acquisition and data analysis. Examples of fielded MS instrumentation for homeland protection will be provided.

Instrumental Innovations for Ion Mobility-Mass Spectrometry*Ion Mobility MS Interest Group*

John A. McLean, presiding

Advances in instrumental arrangements for 2D separations using IM-MS continue to evolve at a rapid rate. A sampling of these include thermostatically controlled separations, different IM pressure regimes, high resolution designs, multiplexed data acquisition capabilities, new ion source designs, and miniaturization, to highlight but a few. Attendant with these advances are unique capabilities and practical limitations. The focus of this workshop will be a discussion of the latest developments in IM-MS instrumentation and theory both in terms of new capabilities and present challenges to be addressed.

Use of the Ion Trap Mass Spectrometer for Undergraduate Research Projects*Ion Trap Mass Spectrometry Interest Group*

Heather Desaire, presiding

Individuals who use ion traps in undergraduate research programs will discuss their successes and challenges in implementing this research grade device into projects that are appropriate for novice researchers. Please plan to participate by sharing your own experiences or asking questions to others who currently work extensively with undergraduates. This workshop will be especially beneficial for future faculty at predominantly undergraduate institutions as well as any existing researchers who wish to learn more about involving undergraduates in their mass spectrometry research.

Acquisition Strategies for Coupling MS to Ultraperformance/Ultrafast LC*LC/MS & Related Topics Interest Group*

J. Will Thompson, presiding

Improved chromatographic performance of ultraperformance or ultrafast liquid chromatography systems is leading to ever-increasing demands on mass spectrometers. Narrow chromatographic peak widths from these systems allows for higher peak capacity for complex sample analysis and faster analysis times for simple mixture separations, often pushing mass spectrometers to their duty cycle limits for quantitative and/or qualitative analyses. This year's LC/MS & Related Topics workshop discussion will focus on data acquisition strategies that are used to best match the duty cycle of mass spectrometers to the chromatography system used.

Challenges in Peptide Fragmentation and Sequencing*Peptide Fragmentation Interest Group*

Bela Paizs and Michael Van Stipdonk, presiding

This workshop attempts to bridge the information gap between researchers pursuing fundamental and statistical studies on peptide fragmentation with those bio-informaticians writing peptide sequencing software. Topics like fragmentation mechanisms (both CID and EC/TD), fragment ion structures, sequence scrambling upon CID, and recent advances in database search based and de novo sequencing will be discussed in detail.

Careers in Mass Spectrometry*Young Mass Spectrometrists Interest Group*

Connell Cunningham, presiding